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Modeling framework for multi-enzyme in-pot processes applied in amine production

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Nowadays multi-enzyme processes are seen as an alternative to assist in the synthesis of complex compounds of industrial interest [1]. In general, a multi-enzyme in-pot process is characterized by the mixture of enzymes that catalyze several reactions in a single pot. In this manner, purification steps of intermediate products may be eliminated. Consequently, it potentially leads to considerable process improvements like increases in the process yield, and reduction in downstream processing and operating costs [2]. In the analysis of these types of processes, mathematical models and computational tools enable a systematic development of multi-enzyme in-pot processes [3].

The aim of this contribution is to present a methodological framework for modeling multi-enzyme in-pot processes in order to formulate reliable models for further applications e.g. optimization, control, prediction. Additionally, the methodology is exemplified stepwise through the production of amines by combining the action of three enzymes in a single reactor [4]. In the applied method, amines are synthesized from ketones by using the first enzyme (transaminase, E.C. 2.6.1.2) together with L-alanine which provides the amino donor (see figure 1). The generated pyruvate, from the first reaction, is reduced by the second enzyme (lactate dehydrogenase, LDH, E.C. 1.1.1.27) to L-lactate. Removing the pyruvate contributes to both driving the reaction to completion and eliminating pyruvate inhibition of the transaminase. The third enzyme (glucose dehydrogenase, GDH, E.C. 1.1.1.47) is added to the system in order to recycle the NADH cofactor [5].

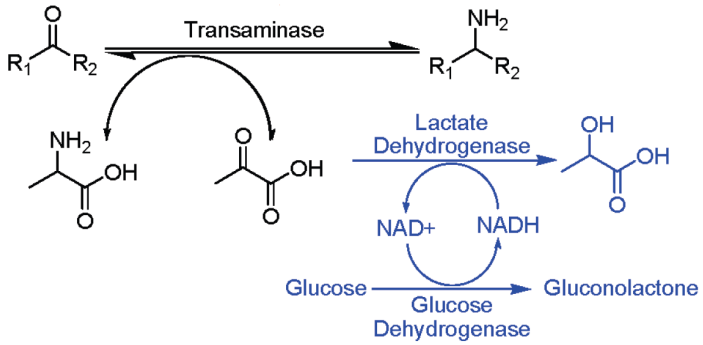

Figure 1. Reaction scheme for the synthesis of amines by applying a three-enzymatic in-pot process (transaminase, LDH and GDH)

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